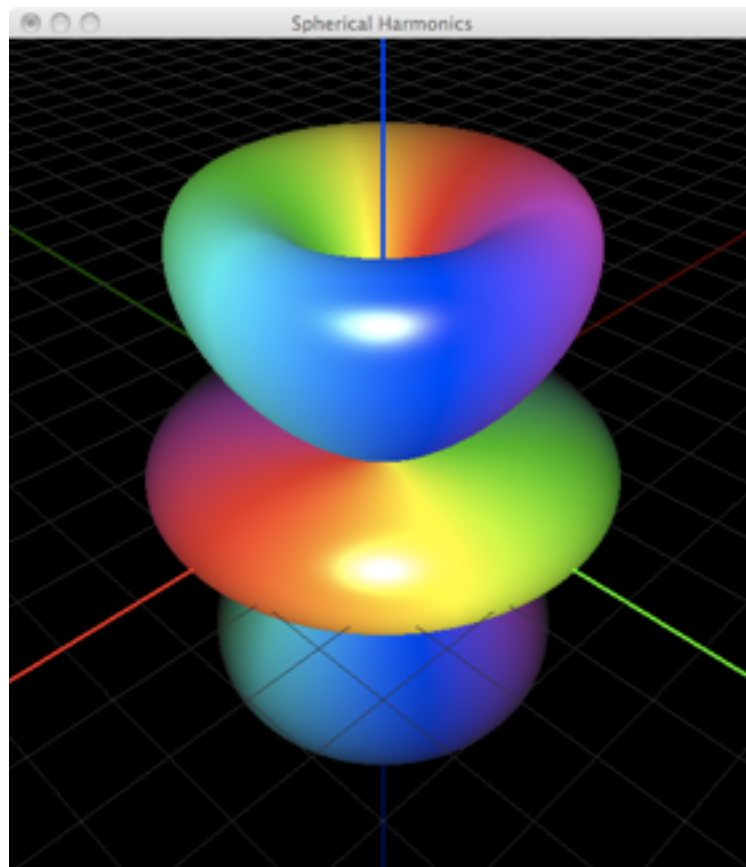
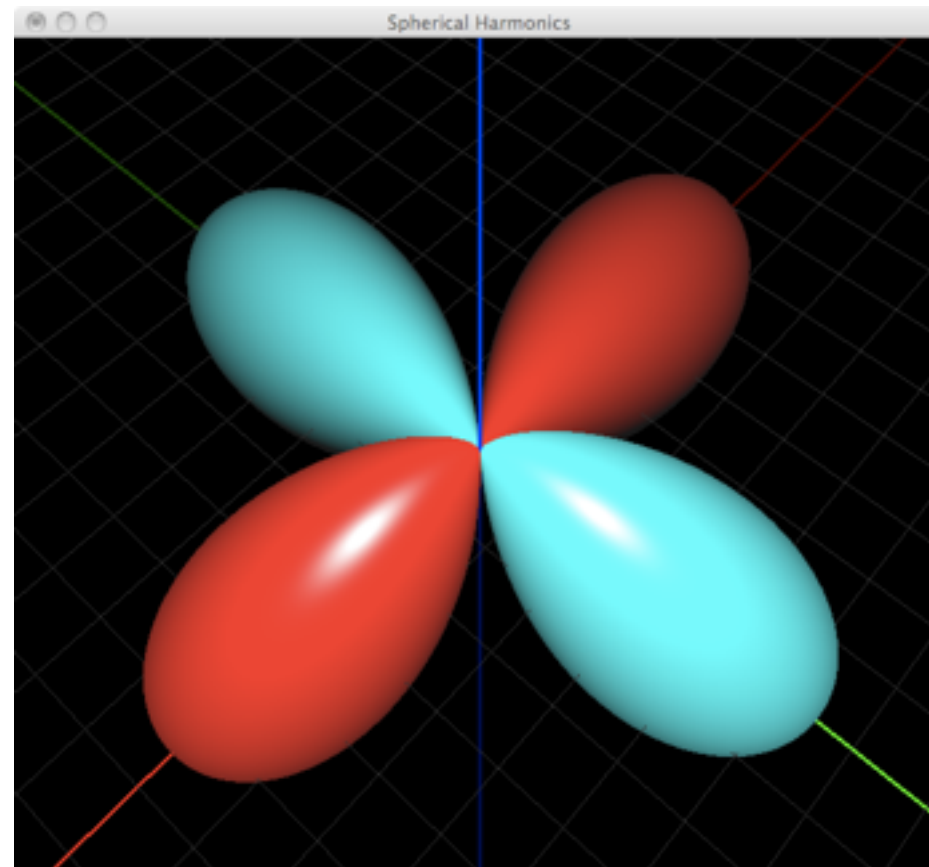
Visualizing Complex Functions using GPUs

Jülich Supercomputing Centre Guest Student Programme 2012

www.cond-mat.de/teaching/JSC/GSP12/

$Y_{3,1}$

d_{x2-y2}

Khaldoon Ghanem

interactive web page

Spherical Harmonics

www.cond-mat.de/teaching/QM/JSim/spherharm.html

Reader

Spherical Harmonics

Polar diagrams of the shperical harmonics: In each direction (ϑ, φ) we plot a point at distance $r = |Y_{l,m}(\vartheta, \varphi)|$ from the origin. We color this point with the phase of $Y_{l,m}(\vartheta, \varphi)$. Connecting these colored points gives the surfaces that are shown. Observe that all spherical harmonics are rotationally symmetric about the z axis, with the phase given by $e^{im\varphi}$. Note: You can rotate and zoom each of the figures to inspect the orbitals.

l=0

m=0

l=1

m=-1 m=0 m=1

l=2

m=-2 m=-1 m=0 m=1 m=2

l=3

m=-3 m=-2 m=-1 m=0 m=1 m=2 m=3

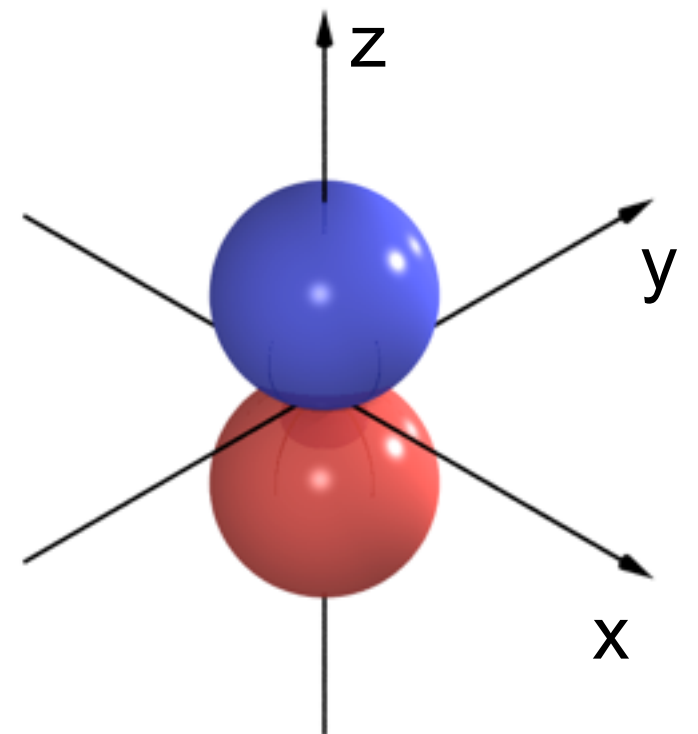
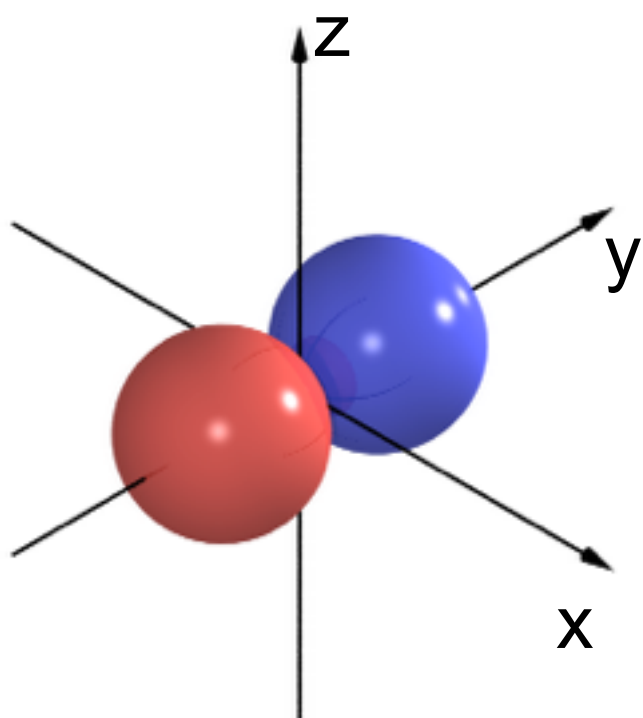
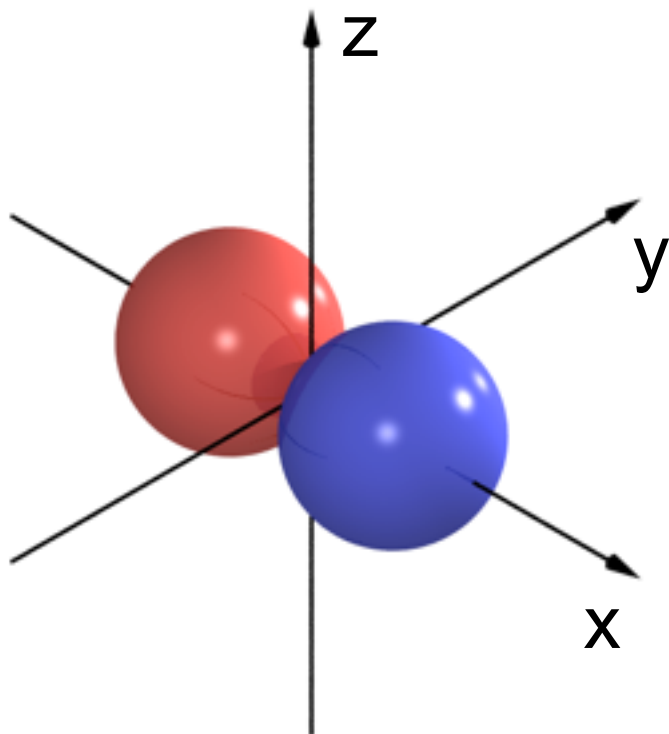
Qian Zhang

p-orbitals (l=1)

real orbitals

$$p_z = Y_{1,0}$$

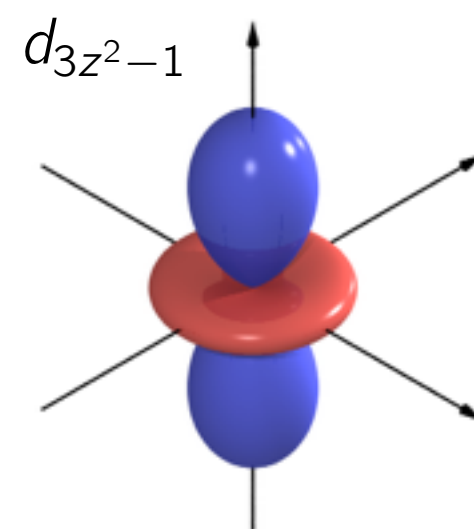
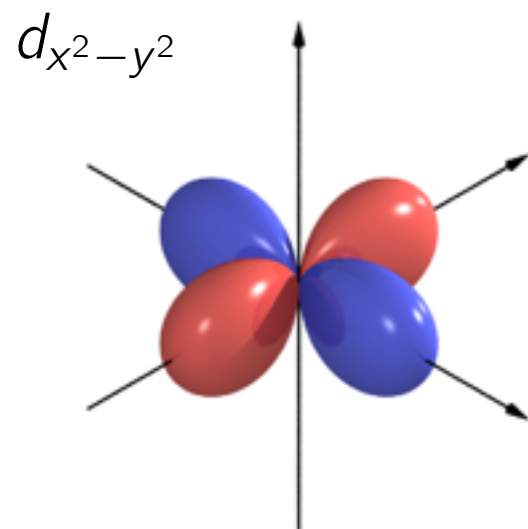
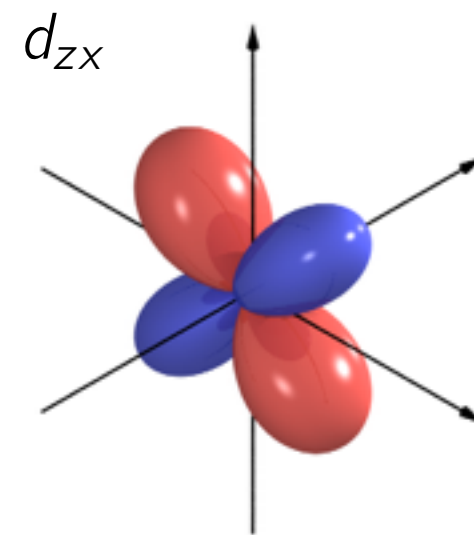
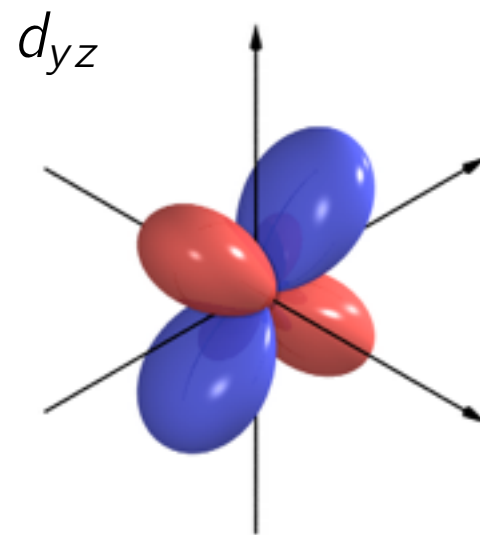
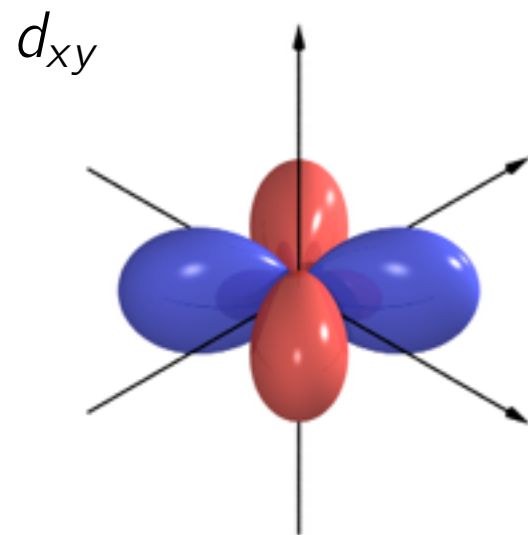
$$p_x = \sqrt{\tfrac{1}{2}}(Y_{1,-1} - Y_{1,1})$$

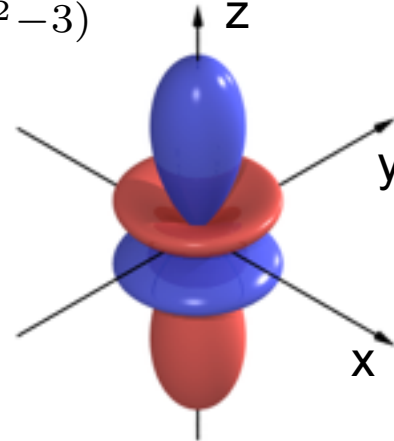
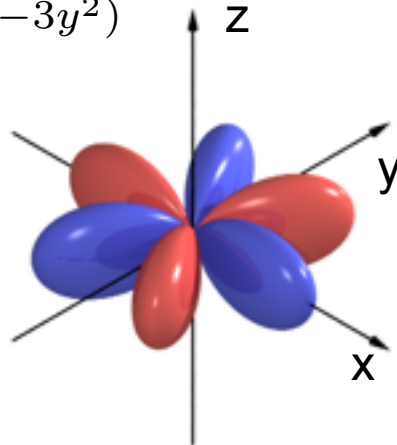
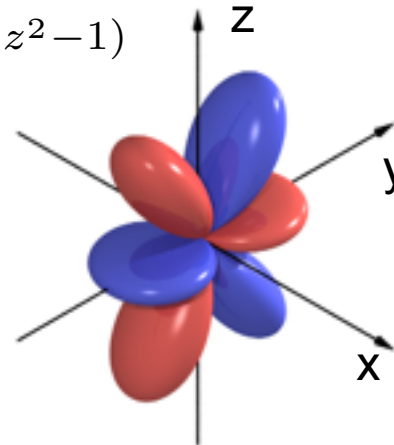
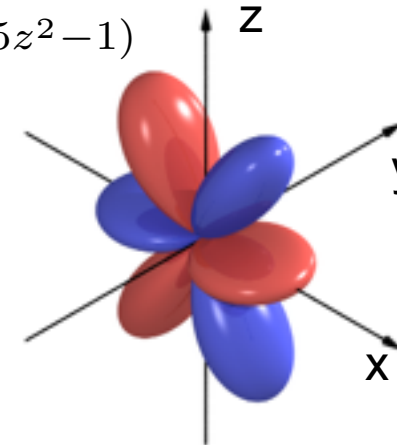
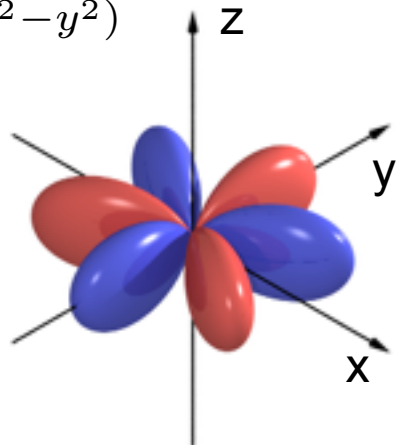
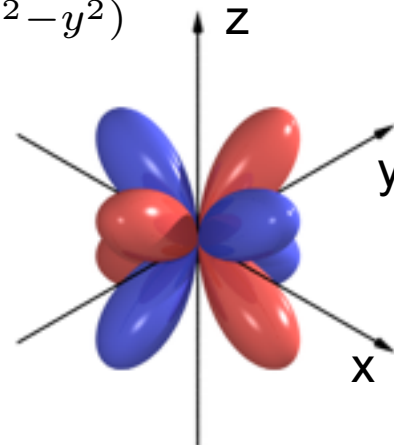
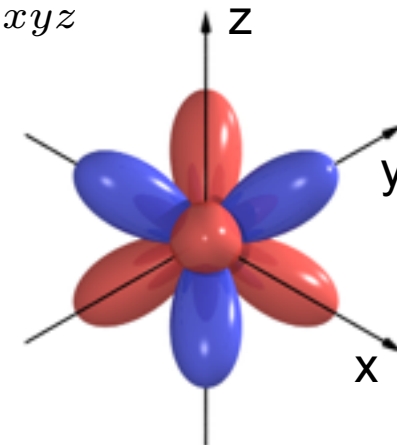
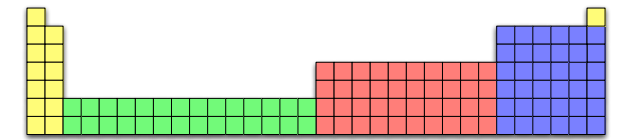
$$p_y = \sqrt{\tfrac{1}{2}}\,i(Y_{1,-1} + Y_{1,1})$$

d-orbitals (l=2)

$$
\begin{array}{lll}
d_{3z^2-1} & Y_{2,0} & \sqrt{\frac{5}{16\pi}}(3\cos^2\theta - 1) \\
d_{zx} & \sqrt{\frac{1}{2}}(Y_{2,-1} - Y_{2,1}) & \sqrt{\frac{15}{16\pi}}\ \sin 2\theta \cos\phi \\
d_{yz} & \sqrt{\frac{1}{2}}i(Y_{2,-1} + Y_{2,1}) & \sqrt{\frac{15}{16\pi}}\ \sin 2\theta \sin\phi \\
d_{xy} & \sqrt{\frac{1}{2}}i(Y_{2,-2} - Y_{2,2}) & \sqrt{\frac{15}{16\pi}}\ \sin^2\theta \cos\phi \\
d_{x^2-y^2} & \sqrt{\frac{1}{2}}(Y_{2,-2} + Y_{2,2}) & \sqrt{\frac{15}{16\pi}}\ \sin^2\theta \sin\phi
\end{array}
$$

d_{xy} d_{yz} d_{zx}

$d_{x^2-y^2}$ d_{3z^2-1}

f-orbitals

$f_{z(5z^2-3)}$
z
y
x

$f_{x(x^2-3y^2)}$
z
y
x

$f_{y(5z^2-1)}$
z
y
x

$f_{x(5z^2-1)}$
z
y
x

$f_{y(3x^2-y^2)}$
z
y
x

$f_{z(x^2-y^2)}$
z
y
x

f_{xyz}
z
y
x

Periodic Table

H																	He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	Lu	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	Lr	Rf	Db	Sg	Bh	Hs	Mt									

La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb
Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No

Periodic Table

1s
1s
2s
2p
3s
3p
4s
3d
4p
5s
4d
5p
6s
5d
6p
7s
6d
4f
5f